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Solvent effects on infrared spectroscopic and calorimetric characteristics of aliphatic ketones in binary solvent mixtures

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Abstract

Solution enthalpies of n-hexane, acetone, butan-2-one and octan-2-one in a series of tetrachloromethane-acetonitrile mixtures and the carbonyl stretching absorption frequencies in the IR spectra of these ketones were determined. It was found that over the whole range of concentrations (varying from neat tetrachloromethane up to neat acetonitrile) the solvation enthalpy of these compounds can be obtained additively from the contributions of the alkyl and carbonyl fragments. The solvent effect on the solvation enthalpy of the carbonyl group was found to be satisfactorily correlated with the corresponding IR frequency shifts of the C=O group. It was also found that the sensitivities of the carbonyl IR frequencies to the solvent composition are different for various ketones. From both IR and calorimetric data, the preferential solvation parameters were evaluated. The differences between the IR spectroscopic and calorimetric data are discussed. © 1998 John Wiley & Sons, Ltd.

Keywords

Calorimetry, IR spectra, Ketones, Solvation